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NITRIC OXIDE PRODUCTION IN LAMINAR AND TURBULENT DIFFUSION FLAM--ETC(U)  
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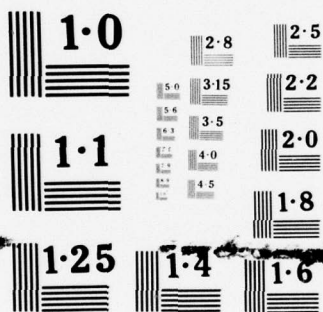
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# NITRIC OXIDE PRODUCTION IN LAMINAR AND TURBULENT DIFFUSION FLAMES

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An analysis of the production of Nitric Oxide in laminar and turbulent diffusion flames has been carried out taking advantage of the large activation energy of the NO producing reactions.

In laminar diffusion flames the NO production takes place in a thin high temperature region adjacent to the thin reaction zone for the main reaction. The mass of NO produced per unit flame surface and time is calculated in terms of the main characteristics of the Burke-Schumann thin flame solution.

The NO production rate in turbulent diffusion flames is related to the probability density function for an inert species diffusing through the mixing region.

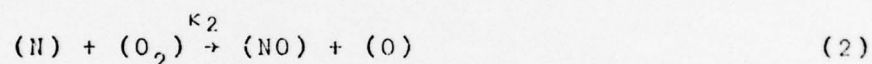
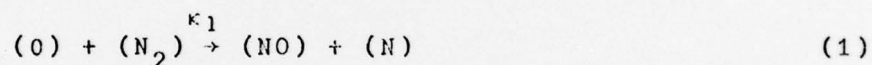
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## I - INTRODUCTION

The production of Nitric Oxide has been analyzed for the laminar diffusion flames associated with fuel droplet combustion by Bracco (1972), Altenkirch et al. (1972) and Kesten (1972). The "NO" production in turbulent diffusion flames has been analyzed, among others, by Fletcher and Heywood (1971), Quang et al. (1972), Kent and Bilger (1972) and (1974) and by Gouldin (1974).

In most of these studies the instantaneous rate of "NO" production has been determined by using the reaction mechanism proposed by Zeldovich (1946)



If the concentration of NO in the region of NO production is small compared with its local equilibrium value the effects of the reverse reactions can be neglected. The rate constant for the second reaction is large compared with that of the first reaction so that the nitrogen atom concentration N can be obtained using the steady state approximation

$$k_1 \{N_2\} \{O\} = k_2 \{N\} \{O_2\} \quad (3)$$

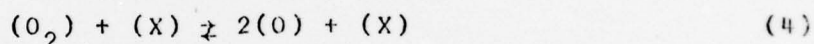
in terms of the molar concentrations of  $N_2$ ,  $O_2$  and O, and, in addition, the production rate of NO in moles/cm<sup>3</sup> sec. is given by

$$\{NO\} = 2k_1 \{N_2\} \{O\} \quad (3a)$$

where  $k_1$ , according to Wray and Teare (1962), is given in cm<sup>3</sup>/mole.sec

by  $k_1 = 7.10^{13} \exp(-38100/T)$ , with  $T$  in  $^{\circ}\text{K}$ .

The rate constant  $k_1$  is very often small compared with those of the reactions between the main reacting species so that the changes in concentrations of  $\text{N}_2$ ,  $\text{O}_2$  and  $\text{O}$  associated with the reactions (1) and (2) can be neglected compared those associated with the main reactions. Very often the reaction rate for the main reaction between the fuel and air is so fast that the concentration of the main reacting species can be calculated using this assumption of local equilibrium. Thus, if the reactions, where (X) is any third molecule,



are assumed in equilibrium, then

$$\{ \text{O} \} / \{ \text{O}_2 \}^{1/2} = 4.1 \exp(-29500/T) (\text{moles/cm}^3)^{1/2} \quad (5)$$

For the temperatures and pressures of interest in many applications the resulting value of  $\{ \text{O} \}$  is very small compared with the concentration of the major species,  $\{ \text{N}_2 \}$ ,  $\{ \text{O}_2 \}$  and the concentration of fuel  $\{ \text{F} \}$ .

The production rate of NO as given by (3) and (5) is

$$\{ \text{NO} \} = 5.74 \times 10^{14} \{ \text{N}_2 \} \{ \text{O}_2 \}^{1/2} \exp(-67600/T) \quad (6)$$

$$w_{\text{NO}} = 1.09 \cdot 10^{14} \rho^{3/2} Y_{\text{N}_2} Y_{\text{O}_2}^{1/2} \exp(-67600/T) \quad (7)$$

in  $\text{grams/cm}^3 \text{ sec}$ . Here  $\rho$  is the density in  $\text{gram/cm}^3$  and  $Y_{\text{N}_2}$  and

$Y_{O_2}$  are the mass fractions of  $N_2$  and  $O_2$ .

The local chemical equilibrium assumption for the reacting species can be used to calculate the local mass fraction of  $O_2$  in terms for example of the mass fraction of the elements, which are conserved by the chemical reactions.

In previous analyses of the production of NO in laminar and turbulent diffusion flames the production rate given above, Eq.(7), was used in connection with the conservation equations for {NO} which were integrated numerically to provide the distribution of {NO}. Here we shall use the fact that reaction rate  $w_{NO}$  is very sensitively dependent on temperature, because the activation temperature  $T_a = 67600^\circ K$  of the reaction rate of Eq.(7) is very large compared with  $T$ , to simplify the analysis of "NO" production in laminar and turbulent diffusion flames.

We shall use the thin flame assumption of Burke Schumann, see Williams (1965), to calculate the distribution of temperature and concentration of the species  $N_2$  and  $O_2$ .

## II - "NO" PRODUCTION IN LAMINAR DIFFUSION FLAMES

In figure 1 we represent schematically the configuration of a typical diffusion flame. A thin flame, where the main reaction between the fuel and the air takes place, separates a region without fuel from a region free from oxygen. Also shown in Fig 1 are typical concentration and temperature profiles corresponding to a cross section BB'.

According to the overall expression for the NO production given above, Eq.(7), this production will only take place at the region immediately adjacent to the thin flame, on the air side,



where the temperature has not decreased much below the adiabatic flame value  $T_f$  corresponding to the infinitely thin flame. When the temperature decreases slightly below  $T_f$ , the NO production becomes negligible because of its large sensitivity with temperature. We have sketched in Fig.1 the region of NO production adjacent to the thin flame.

Because of the small thickness of the region of NO production we may talk about the mass rate of NO produced per unit flame surface  $m''_{NO}$ . Then, we can use this rate as a surface source of NO, located on the thin diffusion flame, when calculating the NO distribution in the flow field.

The mass of NO produced per unit flame surface and time  $m''_{NO}$  is given by

$$m''_{NO} = \int w_{NO} dy \quad (8)$$

where  $y$  is the distance normal to the thin flame, and the integral is extended to the region close to the thin flame where  $w_{NO}$  is significant. To calculate  $m''_{NO}$  we need to know, according to Eq.(7), the temperature and concentration profiles for  $Y_{N_2}$  and  $Y_{O_2}$ ; (the pressure may be assumed to be constant in low speed diffusion flames). However, the NO production will only be significant in a thin region close to the thin flame, and therefore we may, when evaluating the integral in Eq.(6), neglect the small changes in  $\rho$ , and  $Y_{N_2}$  in the NO production zone, using in Eq.(3) their values calculated at the thin flame (subscript  $f$ ). We shall only retain the variation, across the thin production zone, of  $Y_{O_2}$  and of the Arrhenius exponential.

In the thin production zone the mass fraction of  $O_2$  may be approximated by

$$Y_{O_2} = y \frac{\partial Y_{O_2}}{\partial y} \Big|_f = y m_{O_2}'' / \rho_f D_f \quad (9)$$

where  $m_{O_2}''$  is the mass rate of consumption of  $O_2$  per unit flame surface and  $D$  is the diffusion coefficient of  $O_2$  in the mixture. The Arrhenius exponential may be linearized following Frank-Kamenetskii around the value  $T_f$  because  $T_a/T_f = 67600/T_f \gg 1$ . That is we shall write

$$\exp(-T_a/T) \approx \exp(-T_a/T_f) \exp\{T_a(T-T_f)/T_f^2\} \quad (10)$$

where the temperature difference  $(T-T_f)$  in the exponent will be approximated in the production region by

$$T - T_f = y \frac{\partial T}{\partial y} \Big|_f = -y q_{O_2}'' / k_f$$

Here  $q_{O_2}''$  is the heat flux per unit flame surface from the flame toward the oxygen side of the flame, and  $k_f$  is the heat conductivity of the mixture at the thin flame conditions.

As a result of these approximation we obtain, in  $\text{gr/cm}^2 \cdot \text{sec}$ ,

$$m_{NO}'' \approx 1.09 \rho_f^{3/2} Y_{N_2 f} \int_0^\infty Y_{O_2}^{1/2} e^{-T_a/T} dy \approx$$

$$m_{NO}'' \approx 0.96 \cdot 10^{14} \rho_f^{3/2} Y_{N_2 f} \left( \frac{m_{O_2}''}{\rho_f D_f} \right)^{1/2} \left( \frac{q_{O_2}''}{k_f} \frac{T_a}{T_f^2} \right)^{-3/2} e^{-T_a/T_f} \quad (11)$$

This result is obtained as the first approximation when evaluating the integral of Eq.(8) by means of Laplace asymptotic technique for large values of the exponent  $(67600/T_f)$ .

Taking into account the fact that the heat flux  $q''_{O_2}$  will in most cases be proportional to the oxygen mass consumption rate  $m''_{O_2}$ , the NO production rate will then be inversely proportional to  $m''_{O_2}$ .

$$\frac{m''_{NO}}{m''_{O_2}} = 0.96 \cdot 10^{14} e^{-T_a/T_f} \left( \frac{m''_{O_2}}{q''_{O_2}} \right) \left( \frac{c_p T_f^2}{L_e T_a} \right)^{3/2} \left( \frac{\rho_f D_f}{m''_{O_2}} \right)^2 \frac{\rho_f^{1/2}}{D_f} \quad (12)$$

where  $L_e = \rho_f c_p D_f / k_f$  is the Lewis number.

In particular, in the analysis of the quasi-steady burning of fuel droplets of radius  $a$  in air, both  $m''_{O_2}$  and  $q''_{O_2}$  will be proportional to  $a^{-1}$ . On the other hand, the thermodynamic properties at the flame surface are found to be independent of the droplet radius when the Burke-Schumann, thin flame, analysis is used for the main reaction. This analysis can be used to predict the flame characteristics as long as the droplet radius does not become so small that flame extinction occurs. Then

$$m''_{NO} \sim a^{-1/2} a^{3/2} = a,$$

and the ratio  $m''_{NO}/m''_{O_2}$  between the rates of NO production and  $O_2$  or fuel consumption is proportional to  $a$ , indicating the importance of a reduction in droplet size in reducing the NO production.

Notice that  $m''_{NO}$  has been found as a function of the oxygen mass consumption, heat release rate, and other thermodynamic data of the thin diffusion flame corresponding to the main reaction between the fuel and air. All these data can be obtained by using the standard procedures of calculating diffusion flames with the Burke-Schumann assumption.



### III - The production of "NO" in turbulent diffusion flames

When analyzing a turbulent reacting flow we encounter the problem that the fluctuations of the reacting species are of the order of their mean values, so that the mean production rate can not be written in terms of the "laminar reaction rates" or rates calculated using the mean values of the concentration and temperature. This difficulty led Hawthorne, Weddell and Hottel (1949) to the introduction of a probability distribution function for the concentration and a method of calculating the mean product concentration. The probability distribution function has been used later by Toor (1962), O'Brien (1971), Fletcher and Heywood (1971), Kent and Bilger (1972), Rhodes et al. (1973), Bush and Fendell (1973), Lin and O'Brien (1974) and Bilger and Kent (1974). See also the review by Bilger (1976).

We leave for an Appendix the analysis of the turbulent mixing and infinitely fast irreversible reaction of a low speed stream of fuel with air. We show that, under the assumption of equal diffusivities of heat and mass, the instantaneous concentrations and temperature of all the species can be calculated in terms of the instantaneous concentration of one of the species, i.e. molecular oxygen, where it is different from zero.

Thus we obtain the relations

$$\frac{T - T_{20}}{T_{10} + qY_{10}/c_p - T_{20}} - \frac{T - T_{20} + q(Y_2 - Y_{20})/\nu c_p}{T_{10} - T_{20} - qY_{20}/\nu c_p} = 0 \quad (13)$$

$$1 - \frac{Y_{N_2}}{(Y_{N_2})_{20}} - \frac{Y_{20} - Y_2}{\nu Y_{10} + Y_{20}} = 0 \quad (14)$$

between the temperature  $T$ , the Nitrogen mass fraction  $Y_{N_2}$  and the

mass fraction of oxygen  $Y_2$  (for the notation see the Appendix).

We could similarly calculate the mass fraction of all the other species and thus the density if the pressure fluctuations are neglected in the equation of state. We could thus calculate, using Eq.(7), the instantaneous production rate of NO as a function of  $Y_2$ .

If the probability distribution function,  $P_2(Y_2)$ , for the mass fraction of oxygen were known then we could use the instantaneous production rate  $w_{NO}$  to calculate the local mean production rate  $\bar{w}_{NO}$  as

$$\bar{w}_{NO} = \int_0^{Y_2^0} w_{NO}(Y_2) P_2(Y_2) dY_2 \quad (15)$$

To calculate this integral we shall make use of the fact that because  $T_a \gg T$  the NO production is so sensitively dependent on temperature that the local NO production will be limited to those times when the concentration of  $Y_2$  is sufficiently small, so that  $T$  is close to the value  $T_f$  (adiabatic flame temperature) obtained from Eq. (13) by writing  $Y_2 = 0$ . That is

$$\frac{T_f - T_{20}}{T_{10} - T_{20} + qY_{10}/c_p} = \frac{T_f - T_{20} - qY_{20}/vc_p}{T_{10} - T_{20} - qY_{20}/vc_p} \quad (16)$$

when  $Y_2$  is not small so that  $(T_f - T)T_a/T_f^2$  becomes large compared with one, the Arrhenius exponential in  $w_{NO}$  becomes so small that the NO production may be neglected.

Then all the factors entering the integrand of Eq(15) with the exception of  $|O_2|^{1/2}$  and the Arrhenius exponent, can be

taken as constant and evaluated at the condition corresponding to  $Y_2=0$  (and  $Y_1=0$ ) which we shall designate with the subscript f.

Thus we obtain

$$\bar{w}_{NO} = 1.09 \cdot 10^{14} (\rho^{3/2} Y_{N_2})_f P_2(0^+) I \quad (17)$$

where

$$I = \int_0^{Y_{20}} Y_2^{1/2} \exp(-T_a/T) dY_2 \quad (18)$$

To calculate the integral I we can linearize the Arrhenius exponent around the value  $T = T_f$ , and take into account the relation (13) between T and  $Y_2$  written here as

$$T_f - T = (T_{10} - T_{20} + q Y_{10}/c_p) Y_2 / (Y_{20} + v Y_{10}) \quad (19)$$

so that the integral simplifies to

$$I \approx e^{-T_a/T_f} \int_0^\infty Y_2^{1/2} \exp\left(-\frac{T_a}{T_f^2} \frac{(T_{10} - T_{20} + q Y_{10}/c_p) Y_2}{Y_{20} + v Y_{10}}\right) dY_2 \quad (20)$$

where the upper limit in the integral has been replaced by  $\infty$ , because the integrand becomes extremely small when the exponent becomes moderately large compared with one.

Then

$$I = \frac{T_a}{T_f^2} \frac{T_{10} - T_{20} + q Y_{10}/c_p}{Y_{20} + v Y_{10}}^{-3/2} \frac{\sqrt{\pi}}{2} \exp(-T_a/T_f) \quad (21)$$

We have thus obtained the local mean "NO" production rate

in terms of zone thermodynamic data the adiabatic diffusion flame temperature  $T_f$ , and in terms of the particular value  $P_2(0^+, \vec{x})$  of the probability distribution function of  $Y_2$ . According to Eq.(20) of the appendix

$$P_2(0^+, \vec{x}) = \frac{1}{Y_{20} + vY_{10}} P\left(\frac{Y_{20}}{Y_{20} + vY_{10}}, \vec{x}\right), \quad (22)$$

so that the NO production is thus given in terms of this particular value, at  $Y=f_c$ , of the probability distribution function for an inert species, of unit concentration in the fuel stream and zero concentration in the air stream.

The fact that the production of Nitric Oxide is dependent, not on smooth moments, but on the detailed shape of the probability distribution function for an inert species, illustrates the need for measurements and theories providing this p.d.f.. The measurements of the p.d.f. in a two-dimensional turbulent mixing layer by Rebollo(1972) show that these functions are not Gaussian but some-times approach bimodal distributions.



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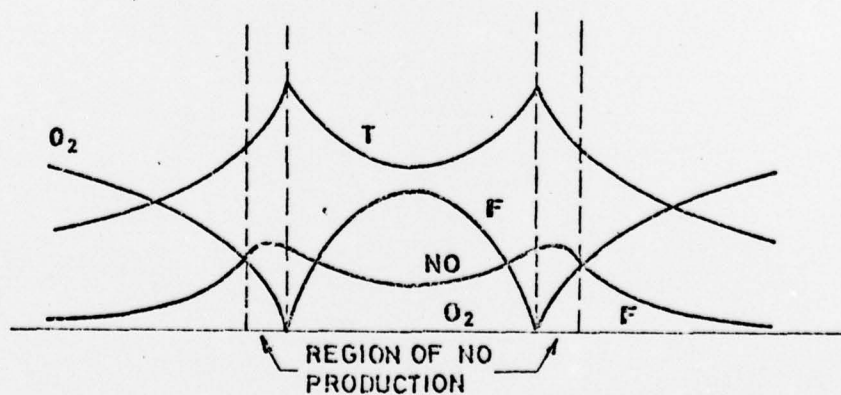
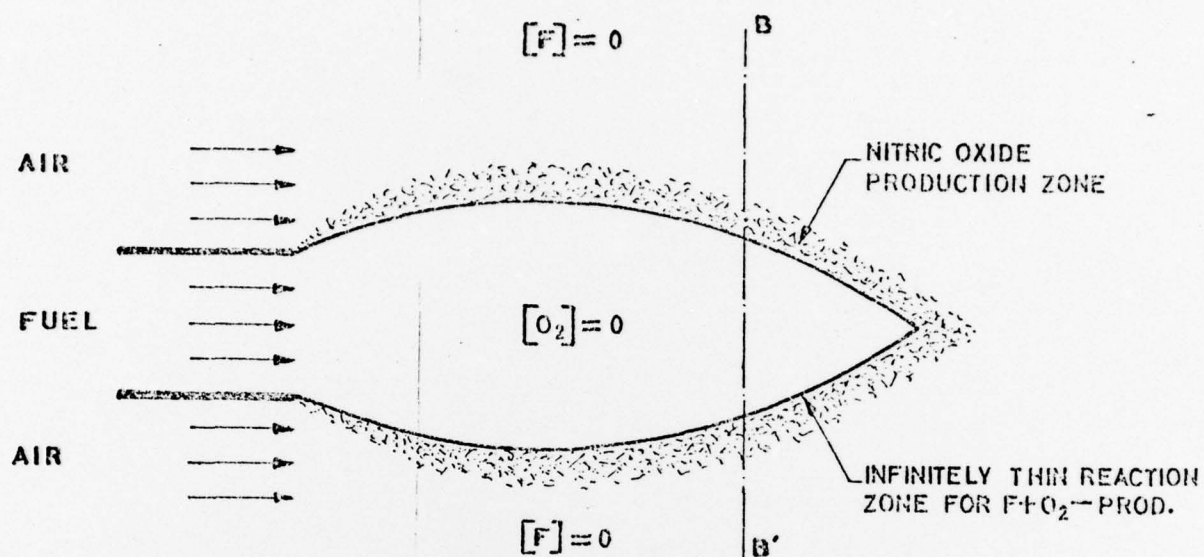


FIG.1

## A P P E N D I X

"THE ROLE OF THE PROBABILITY DISTRIBUTION FUNCTION FOR THE CONCENTRATION OF AN INERT SPECIES IN THE ANALYSIS OF TURBULENT DIFFUSION FLAMES".

- - - - -

We shall analyze in this Appendix some aspects of the turbulent mixing and chemical reaction between two reactants undergoing a one-step irreversible reaction of the form



We shall assume that the molecular diffusion velocities are related to the instantaneous concentration field by Fick's law with equal diffusion coefficients  $D$  for all the species. We shall assume that the specific heats of all the species are equal to  $c_p$ , and constant. In addition, we shall limit the analysis to low speed flows, for which the viscous dissipation and the work associated with pressure gradients can be neglected. We shall consider the thermal diffusivity to be equal to  $D$ .

With these assumptions, the instantaneous temperature and concentration field will satisfy the following conservation equations

$$L(Y_i) = w_i \quad (2)$$

$$L(c_p T) = -w_1 q + \frac{\partial p}{\partial t} \quad (3)$$

where  $L$  is the operator

$$L(Y) = \frac{\partial}{\partial t} (\rho Y) + \nabla \cdot (\rho \vec{v} Y) - \nabla \cdot (\rho D \nabla Y) \quad (4)$$

In these equations  $Y_i$  is the mass fraction of species  $i$ ,  $\rho$  the density,  $T$  the temperature,  $p$  the pressure,  $\vec{v}$  the velocity, and  $w_i$  is the mass production rate of species  $i$  per unit volume.

If we take into account the overall stoichiometric relation (1) we can write

$$w_1 = w_2/v = -w_3/(1 + v) \quad (5)$$

where  $v = p_2 M_2 / M_1$  is the stoichiometric mass ratio oxygen (species 2) to fuel (species 1).  $M_i$  is the molecular mass of species  $i$ . For an inert species  $j$ ,  $w_j = 0$ .

In Eq.(3),  $q$  is the heat release per unit mass of fuel, or

$$q = h_1^0 + v h_2^0 - (1 + v) h_3^0 \quad (6)$$

in terms of the specific heats of formation of the reacting species and products.

Notice that the conservation equations (2) and (3) are valid for turbulent flow as long as we use in them the instantaneous values for  $\vec{v}$ , the thermodynamic variables and  $w_i$ .

There are many reactions that can be described by an overall reaction of the form (1) only if the characteristic mechanical time, in this case given by the smaller time scale of the turbulent flow, is large compared with some characteristic chemical time as required, for example, to establish a stationary state in the radical concentrations.

From the conservation equations (2) and (3), we deduce, if Eq.(5) is taken into account that

$$L(Y_2 - vY_1) = 0 \quad (7)$$

$$L(Y_3 + (1 + v)Y_1) = 0 \quad (8)$$

$$L(T + qY_1/c_p) = 0 \quad (9)$$

so that the combinations

$$(Y_2 - vY_1), \{Y_3 + (1 + v)Y_1\} \text{ and } (T + qY_1/c_p)$$

obey the same equation as an inert species. For Eq.(9) to be valid the term  $\partial p/\partial t$  in Eq.(3) should be negligible. This is the case for low speed flows if the mean pressure outside the mixing zone does not vary with time.

For species 1 we must use an equation

$$L(Y_1) = w_1 \quad (10)$$

where the chemical production term must be retained. If, however, we consider cases for which the characteristic chemical time for the reaction (1) is short compared with the smaller time scale of the turbulent flow, we can then substitute Eq.(10) by

$$w_1 = 0 \quad (11)$$

or taking into account the overall irreversibility of the reaction (1), by

$$Y_1 Y_2 = 0 \quad (12)$$

showing that the fuel and oxygen do not coexist anywhere in the flow field.



Eq.(12), together with the conservation Eqs.(7) to (9), a conservation equation

$$L(Y_j) = 0 \quad (13)$$

for the inert species, and the momentum equation

$$\frac{\partial \rho \vec{v}}{\partial t} + \nabla \cdot (\rho \vec{v} \vec{v}) = - \nabla p + \rho \vec{f}_m + \nabla \cdot \tau_v \quad (14)$$

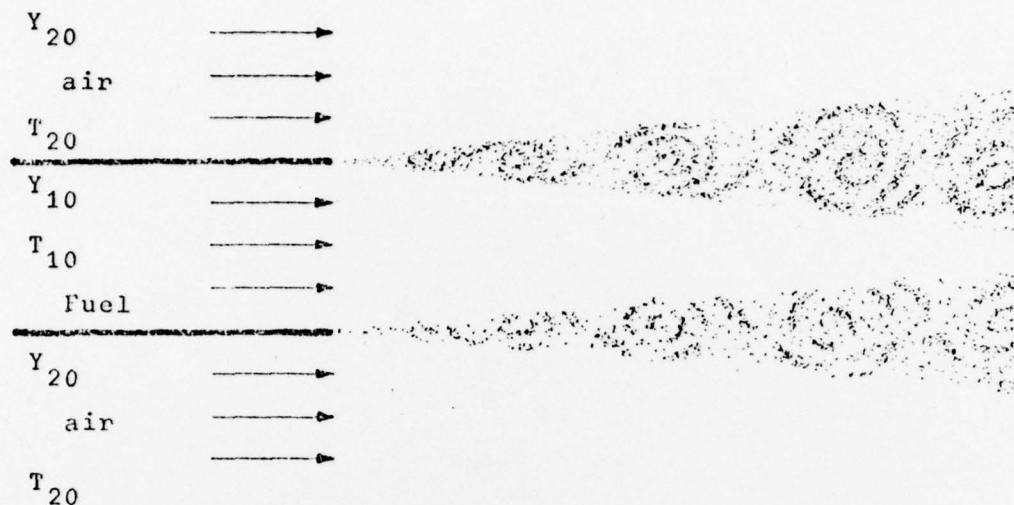
and equation of state

$$P = \rho TR(\sum Y_i / M_i) \quad (15)$$

when used with appropriate initial and boundary conditions would determine the instantaneous velocity, temperature and concentration fields. Because the reaction rates do not appear in these equations the reaction is called diffusion controlled.

These equations are to be solved with appropriate initial and boundary conditions. If the resulting flow is turbulent, this is a formidable problem. Our purpose here is to show how we can obtain information for the distribution of concentrations and temperature in diffusion controlled combustion from details of the concentration distribution for an inert species. In addition there are cases where the heat release associated with combustion will not affect much the turbulent flow. In these cases, appropriate experiments in turbulent mixing without combustion can be used to calculate the temperature and concentration distributions in diffusion controlled combustion.

Let us consider, for example, the turbulent mixing of a jet of fuel with a co-flowing stream of air, as shown in figure 1,



and let us assume that we know the concentration  $Y$  of an inert species, of unit concentration in the incoming stream of fuel, and zero concentration in the air.

Thus  $Y$  is a random function  $f_a(\vec{x}, t)$ , which we shall describe in terms of the probability distribution function  $P(Y, \vec{x})$ . If the overall process is stationary the time will not appear in this function. This function is such that  $P(Y, \vec{x})dY$  is the probability of having at the point  $\vec{x}$  a concentration of the inert species between  $Y$  and  $Y + dY$ .

Now, the combinations

$$f_1 = \frac{-Y_2 + vY_1 + Y_{20}}{vY_{10} + Y_{20}} \quad , \quad f_2 = \frac{Y_3 + (1+v)Y_1}{(1+v)Y_{10}} \quad \text{and}$$

$$f_3 = \frac{T + qY_1/c_p - T_{20}}{T_{10} + qY_{10}/c_p - T_{20}} \quad , \quad f_4 = \frac{Y_2 + vc_p T/q - vc_p T_{20}/q - Y_{20}}{-Y_{20} + vc_p T_{10}/q - vc_p T_{20}/q} \quad (16)$$

satisfy the same transport equation and boundary conditions as the inert species Y, so that they have the same probability distribution function. That is,  $P(f_1, \vec{x}) df_1$  is the probability of having the combination  $(vY_1 + Y_{20} - Y_2)/(vY_{10} + Y_{20})$  take a value between  $f_1$  and  $f_1 + df_1$ .

If we now take into account the equilibrium relation (12), we can now obtain the probability distribution function for the species  $Y_1$ ,  $Y_2$  and  $Y_3$  and for the temperature T.

Thus to calculate the probability distributions function  $P_1(Y_1, \vec{x})$  for  $Y_1$ , we make use of the fact that at times when  $Y_1 \neq 0$  we have  $Y_2 = 0$ , and then the combination  $f_1$  given in (16) is a function of  $Y_1$ :  $f_1 = (vY_1 + Y_{20})/(vY_{10} + Y_{20})$  for whom we know the probability distribution function  $P(f_1, \vec{x})$ . When  $Y_1$  lies between  $Y_1$  and  $Y_1 + dY_1$ ,  $f_1$  lies between the corresponding value of  $f_1$  and  $f_1 + (v dY_1)/(vY_{10} + Y_{20})$

so that

$$P_1(Y_1, \vec{x}) = P\left(\frac{vY_1 + Y_{20}}{vY_{10} + Y_{20}}, \vec{x}\right) \frac{v}{vY_{10} + Y_{20}} \quad (17)$$

if  $Y_1 \neq 0$

when  $Y_1 = 0$ ,  $f_1 = (Y_{20} - Y_2)/(Y_{20} + vY_{10}) < f_c$

where

$$f_c = Y_{20}/(Y_{20} + vY_{10}) \quad (18)$$

and the probability of having, at a given point  $\vec{x}$ , a value of  $f_1$  lower than  $f_c$ , that is  $Y_1 = 0$ , is



$$\int_0^{f_c} P(Y, \vec{x}) dY$$

Then we may write the probability distribution function  $P$ , for  $Y_1$  as

$$P_1(Y_1, x) = \frac{v}{vY_{10} + Y_{20}} P\left(\frac{vY_1 + Y_{20}}{vY_{10} + Y_{20}}, \vec{x}\right) + \left\{ \int_0^{f_c} P(Y, \vec{x}) dY \right\} \delta(Y_1) \quad (19)$$

Where the first term gives the probability of having a value of  $Y_1 \neq 0$ , and the last term involving the Dirac  $\delta$  function is the probability of having  $Y_1 = 0$ .

In a similar way

$$P_2(Y_2, \vec{x}) = \frac{1}{Y_{20} + vY_{10}} P\left(\frac{Y_{20} - Y_2}{Y_{20} + vY_{10}}, \vec{x}\right) + \left\{ \int_{f_c}^1 P(Y, \vec{x}) dY \right\} \delta(Y_2) \quad (20)$$

To obtain the probability distribution function for the temperature  $P_T(T, \vec{x})$ , we take into account that at times where  $Y_1 = 0$

$$0 < f_3 = \frac{T - T_{20}}{T_{10} - T_{20} + qY_{10}/c_p} < f_c$$

with  $T$  ranging from  $T_{20}$  to  $T_f$ . And at times where  $Y_2 = 0$

$$1 > f_4 = \frac{T - T_{20} - qY_{20}/v c_p}{T_{10} - T_{20} - qY_{20}/v c_p} > f_c$$

with  $T$  ranging from  $T_{10}$  to  $T_f$

and

$T_f = T_{20} + (T_{10} - T_{20} + qY_{10}/c_p)f_c$  is the adiabatic flame temperature. So that  $P_T = P_{T2} + P_{T1}$  (21)

with

$$P_{T2}(T, \vec{x}) = \frac{1}{T_{10} - T_{20} + qY_{10}/c_p} P\left(\frac{T - T_{20}}{T_{10} - T_{20} + qY_{10}/c_p}, \vec{x}\right) \quad (21a)$$

for  $0 < (T - T_{20})/(T_{10} - T_{20} + qY_{10}/c_p) < f_c$

and  $P_{T2} = 0$ , outside the interval  $(T_{20}, T_f)$

and

$$P_{T1}(T, \vec{x}) = \frac{1}{T_{20} - T_{10} + qY_{20}/vc_p} P\left(\frac{T - T_{20} - qY_{20}/vc_p}{T_{10} - T_{20} - qY_{20}/vc_p}, \vec{x}\right) \quad (21b)$$

for

$1 > (T - T_{20} - qY_{20}/vc_p)/(T_{10} - T_{20} - qY_{20}/vc_p) > f_c$

and  $P_{T1} = 0$ , outside the interval  $(T_{10}, T_f)$

In a similar way we could write the probability distribution function for the product species  $Y_3$ .

The probability distribution function for the temperature could also be obtained as follows. We first notice that the combination

$$\alpha = \frac{T + qY_1/c_p - T_{20}}{T_{10} + qY_{10}/c_p - T_{20}} - \frac{T - T_{20} + q(Y_2 - Y_{20})/vc_p}{T_{10} - T_{20} - qY_{20}/vc_p} \quad (22)$$

diffuses like an inert species, satisfying the differential equation  $L(\alpha) = 0$  with the homogeneous boundary conditions  $\alpha = 0$  so that the solution is  $\alpha = 0$ . That is,

$$\frac{T + qY_1/c_p - T_{20}}{T_{10} + qY_{10}/c_p - T_{20}} - \frac{T - T_{20} + q(Y_2 - Y_{20})/vc_p}{T_{10} - T_{20} - qY_{20}/vc_p} = 0 \quad (23)$$

is a relation between the instantaneous values of  $T$ ,  $Y_1$  and  $Y_2$ . In a similar way we may obtain the following relation

$$\frac{Y_3 + (1+v)Y_1}{(1+v)Y_{10}} - \frac{Y_{20} - Y_2 + vY_1}{Y_{20} + vY_{10}} = 0 \quad (24)$$

between the instantaneous values of  $Y_1$ ,  $Y_2$  and  $Y_3$ , which would enable us to calculate the probability distribution functions  $P_1$  and  $P_2$  given by (19) and (20).

Also, if  $Y_j$  is an inert species, of zero concentration in the fuel stream and concentration  $Y_{jo}$  in the air stream, its probability distribution function  $P_j(Y_j, \vec{x})$  would be given by

$$P_j(Y_j, \vec{x}) = \frac{1}{Y_{jo}} P\left(1 - \frac{Y_j}{Y_{jo}}, \vec{x}\right) \quad (25)$$

a result which can also be obtained from the fact that the instantaneous values of  $Y_1$ ,  $Y_2$  and  $Y_j$  satisfy the relation

$$1 - \frac{Y_j}{Y_{jo}} - \frac{vY_1 + Y_{20} - Y_2}{vY_{10} + Y_{20}} = 0 \quad (26)$$

and using the probability distribution functions given by (19) and (20).

It is interesting to notice that the relations (23), (24) and (26) give  $T$ ,  $Y_3$  and  $Y_j$  in terms of  $T_2$ , at times when  $Y_1 = 0$ , and similar in terms of  $Y_1$  at times when  $Y_2 = 0$ . The mean concentrations  $\bar{Y}_1$ ,  $\bar{Y}_2$ ,  $\bar{Y}_3$  and  $\bar{T}$  can now be obtained as a function of  $\vec{x}$  taking into account the probability distribution functions which have been obtained above. Thus

$$\bar{Y}_2(\vec{x}) = \int_0^{Y_{10}} Y_1 P_1(Y_1, \vec{x}) dY_1 = \int_c^1 \{(Y_{10} + Y_{20}/v)Y - Y_{20}/v\} P(Y) dY \quad (27)$$

$$\bar{Y}_2(\vec{x}) = \int_0^{Y_{20}} Y_2 P_2(Y_2, \vec{x}) dY_2 = \int_c^f \{Y_{20} - Y(Y_{20} + vT_{10})\} P(Y) dY \quad (28)$$

The mean values of  $Y_3$  and  $T$  can be obtained more directly from (23) and (24) which, obviously, are also valid for the mean values.

In conclusion, if we are able to obtain either experimentally or theoretically the probability distribution function  $P(Y, \vec{x})$  for an inert species of normalized concentration  $Y$ , such that it is unity in the fuel stream and zero in the air stream, then, using the ideas given above we can calculate the probability distribution function for the reacting species as well as for the temperature if the following main assumption can be used:

- a) Equal thermal and mass diffusivities for all the species
- b) Infinite reaction rate with an irreversible reaction.



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